FINAL REPORT

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The Role of Turbulence in Chemical and Dynamical Processes in the Near-Field Wake of Subsonic Aircraft

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Abstract

During this grant, covering the period from September 1998 to December 2001, we continued the investigation of the role of turbulent mixing in the wake of subsonic aircraft initiated in 1994 for NASA's Atmospheric Effects of Aviation Project. The goal of the research has been to provide sufficient understanding and quantitative analytical capability to assess the dynamical, chemical, and microphysical interactions in the near-field wake that have the greatest potential to influence the global atmospheric impact of the projected fleet of subsonic aircraft. Through large-eddy simulations we have shown that turbulence in the early wake dynamics can have a strong effect on both the ice microphysics of contrail evolution and on wake chemistry.

The wake vortex dynamics are the primary determinant of the vertical extent of the contrail; this together with the local wind shear largely determines the horizontal extent. The fraction of the initial ice crystals surviving the wake vortex dynamics, their spatial distribution, and the ice mass distribution are all sensitive to the aircraft type, assumed initial ice crystal number, and ambient humidity and turbulence conditions. Our model indicates that there is a significant range of conditions for which a smaller aircraft such as a B737 produces as significant a persistent contrail as a larger aircraft such as a B747, even though the latter consumes almost five times as much fuel.

Large-eddy simulations of the near wake of a B757 provided a fine-grained chemical-dynamical representation of simplified NO_x - HO_x chemistry in wakes of ages from a few seconds to several minutes. By sampling the simulated data in a manner similar to that of *in situ* aircraft measurements it was possible to provide a likely explanation for a puzzle uncovered in the 1996 SUCCESS flight measurements of OH and HO_2. The results illustrate the importance of considering fluid dynamics effects in interpreting chemistry results when mixing rates and species fluctuations are large, and demonstrate the feasibility of using 3D unsteady LES with coupled chemistry to study such phenomena.

Introduction

In 1994 we initiated the development of a wake simulation model for NASA's Atmospheric Effects of Aviation Project. The goal of the research has been to provide sufficient understanding and quantitative capability to assess the dynamical, chemical, and microphysical interactions in the near-field wake that have the greatest potential to influence the global atmospheric impact of the projected fleet of subsonic aircraft. A model was designed to explicitly include the most important turbulent eddies governing the development of the wake from a few seconds after the aircraft until the complete breakup of the trailing vortex system. Its development and preliminary results were described in Lewellen and Lewellen (1996). The model was compared with ground-based lidar measurements of a B737 made during the SNIF field tests by the Aerosol Research Branch at NASA Langley during 1996. A joint paper with the experimenters (Lewellen et al., 1998) showed a good correlation between the lidar observed aerosol emitted from the engines and the model results of a simulated tracer added to the engine emissions.

Based on the above results and some preliminary wake chemistry results (Lewellen and Lewellen, 1997), we received a second grant to continue our wake simulation studies. This second grant included tasks to both use our model to help interpret data collected in the field missions, and to improve upon the model by incorporating ice microphysics to allow more rigorous simulations of the evolution of visible contrails. The added emphasize on ice microphysics was motivated by studies that indicated that the greatest uncertainty surrounding the potential impact of aviation on the atmosphere were probably connected with the potential radiational influence of persistent contrails (Penner et al., 1999).

This current report provides copies of the major publications during the period of this second grant (1998-2001), summarizes the accomplishments, and provides some recommendations for follow on work.

Summary of Accomplishments

Most of he major accomplishments are included in our two journal publications: Lewellen and Lewellen (2001a), included in this document as Appendix A; and Lewellen and Lewellen (2001b), included as Appendix B.

In Lewellen and Lewellen (2001a) we described our incorporation of simplified ice microphysics into the LES wake model and detailed simulations that confirmed that the early wake dynamics can have a strong influence on the properties of persistent contrails even at late times. The most important effect of the aircraft is to provide ice crystals where they might not otherwise be present, ice nucleation proceeding easily following the formation of droplets in the early water-saturated jet exhausts. The aircraft wake dynamics affects the contrail evolution in at least three ways: it largely governs the vertical and horizontal dispersion of the engine exhausts; the low pressure in the vortex correspondingly increases the relative humidity there; and the rapid descent of the vortex system can evaporate some or all of the ice crystals via adiabatic compression.

In these simulations we found that the ice crystal number densities generally remained high enough that the ice is near thermodynamic equilibrium within most of the contrail during its early evolution. The bulk of the total ice mass comes not from the engine exhausts, but from the ambient air supersaturated with respect to ice. Consequently, the ice mass grows proportionally with plume volume, which in turn is largely determined by vortex dynamics, until ~ 4 min, and Brunt-Vaisala oscillations until ~ 20 min. The loss of ice crystals induced by the vortex descent effectively raises the level of supersaturation in the atmosphere required for the production of significant persistent contrails, though by an amount that depends on many factors. The fraction of ice crystals lost through this mechanism depends on a competition between the rate of descent of the vortex system and the rate of mixing between the fluid in the wake and the supersaturated ambient atmosphere. This involves the full 3D wake vortex dynamics, depending on aircraft type as well as on the ambient relative humidity, turbulence level, shear, and stratification. Consequently, the simple assumption often made that ice mass in a contrail for given ambient conditions is proportional to fuel usage is not true in general; a B737, for example, can give rise to as significant a persistent contrail as a

B747, burning ~5 times as much fuel, under conditions with moderate ambient ice supersaturation.

In Lewellen and Lewellen (2001b), we illustrated the importance of considering fluid dynamics effects in interpreting chemistry results when mixing rates and species fluctuations are large, and demonstrated the feasibility of using 3D unsteady LES with coupled chemistry to study such phenomena. A large-eddy simulation of the near wake of a B757, under conditions representative of those found during the SUCCESS mission, provided a fine grained chemical-dynamical representation of simplified NO_x - HO_x chemistry in wakes for ages from a few seconds to several minutes. By sampling this simulated data in a manner similar to that of *in situ* aircraft measurements it was possible to interpret results obtained at the typical sampling rate of 1 Hz. In particular, comparison of these simulation results with actual *in situ* flight measurements of OH and HO_2 performed under cruise conditions during SUCCESS in May of 1996 provide a likely explanation for the apparent large discrepancy between measurement and theoretical expectation found by Tan et al. (1998). The discrepancy appears to be due to two effects of the wake dynamics on the measured chemistry: (1) the effect of averaging over species fluctuations on a scale smaller than can be resolved by the sampling rate, and (2) large turbulent mixing rates near the plume edges dramatically modifying the local equilibrium chemistry predictions. Both are accentuated by the dramatic difference in HO_2 concentration inside and outside of the wake plume.

In as yet unpublished work (assisted by Prof. Wade Huebsch, also of WVU), we have recently improved upon the simplified ice microphysics of Lewellen and Lewellen (2001a) by incorporating into the LES code the more detailed ice microphysics of the NASA Ames Community Aerosol and Radiation Model for Atmospheres (CARMA) code supplied to us by Eric Jensen. This microphysics code has been used for a number of previous contrail and cirrus studies (e.g., Jensen, et al., 1998, and Gierens and Jensen, 1998). Rather than depending upon a single representative ice crystal size at each model grid point in time and space, as in the simplified bulk model, CARMA includes a model specified number of separate crystal size bins in which the particles are allowed to evolve. Incorporating this microphysics in the 3D wake simulations roughly doubles the computer resources (memory and CPU) required; we ported our codes to a larger computer in order to handle this. The qualitative effects of the aircraft wake dynamics on contrail development described in Lewellen and Lewellen 2001a are confirmed in simulations with the more sophisticated ice microphysics; there are, as one would expect, some qualitative differences, however.

Figure 1 illustrates the type of differences in particle size distributions that are obtained. Simulations of *in situ* flight measurement of ice crystal size spectra have been made by calculating the size distribution within a periodic length of a simulated wake. Some resultant size spectra generated by a simulation incorporating the CARMA microphysics using 12 bins are compared with spectra from the simplified bulk model. Both simulations are initially started with the same total ice crystal number and ice mass.

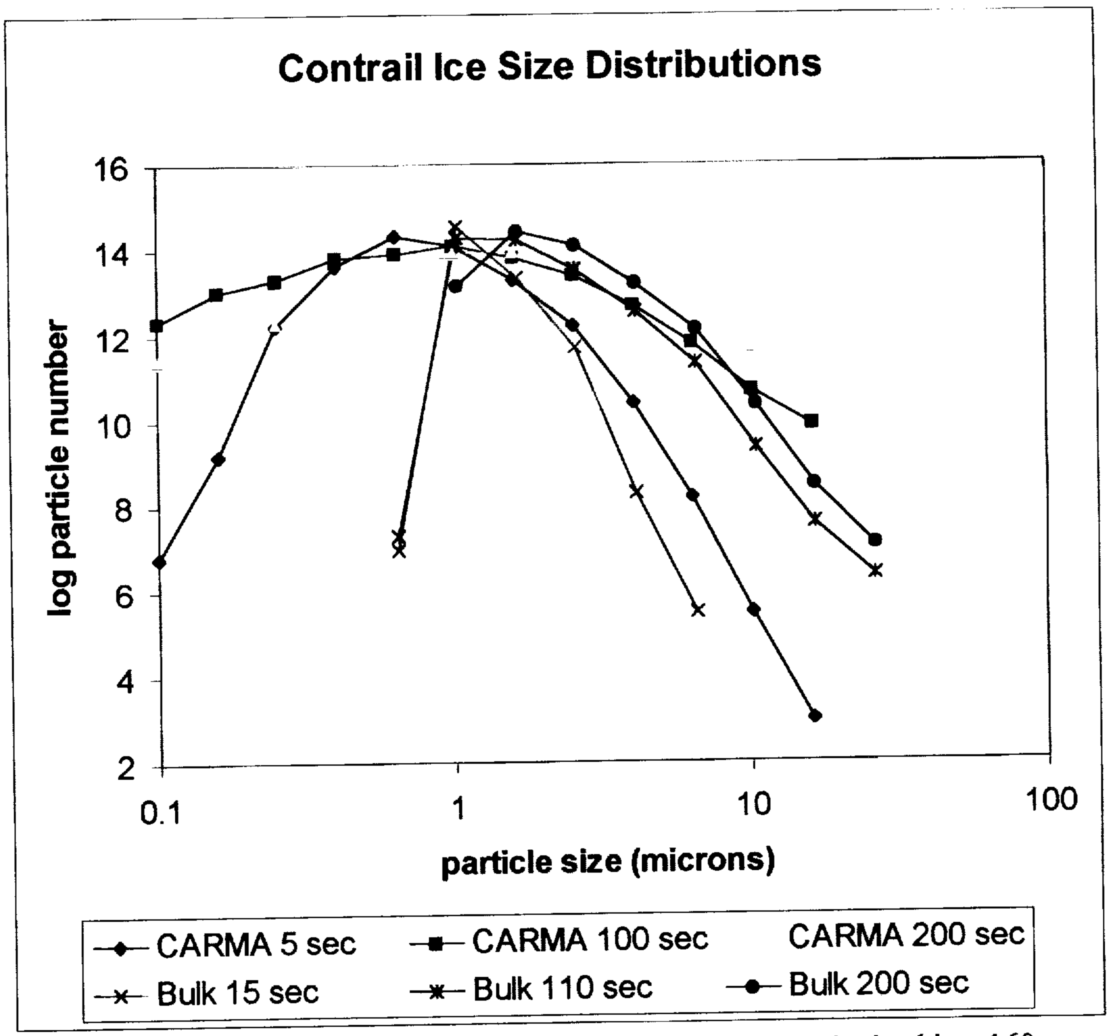

Figure 1. Comparison between the particle size spectra obtained in a 160 m length of LES simulated contrail using either CARMA or bulk microphysics at different times behind a B737 with an ambient 130% supersaturation with respect to ice.

As should be expected the refined microphysics of CARMA provides a broader spectrum with evolving time than that obtained with the previous bulk microphysics. The differences in ice crystal size spectrum between the two models are fairly modest in the early evolution of larger particles, but significant in the larger number of small crystals realized. The difference may be expected to increase as the wake ages and the ice particles in the edges of the wake grow sufficiently large for precipitation to become important.

At medium to high ambient ice supersaturation levels, the evolution of the total contrail ice mass and its spatial distribution proves fairly insensitive to the choice of ice microphysics. The binned microphysics produces only modestly larger (~10%) total ice mass than the bulk microphysics. The difference arises in the upper part of the contrail where crystal densities are lower, crystal sizes larger, and the ice mass has not yet grown to its equilibrium level; the crystals of larger than mean size allowed by the binned microphysics grow at a faster rate, producing the modest enhancement in ice mass.

The loss of ice crystals due to adiabatic heating of the contrail as the vortex dominated portion of the wake is propelled downwards is impacted more significantly. As discussed in Lewellen and Lewellen 2001a, this effect is very sensitive to crystal size and is partly offset by mixing of moist ambient air into the wake as it transports downward. A significant drawback of the simple bulk microphysics is that mixing processes effectively artificially narrow the ice crystal spectrum: mixing a parcel with small crystals and another with large crystals results in a parcel with "medium" crystals. The binned microphysics properly follows the crystal spectrum through mixing events. This is largely responsible for the broader spectrum across the contrail as a whole seen in figure 1. The smaller crystals are more easily evaporated by the adiabatic heating in the dropping wake, increasing the losses due to this effect over what was found for the bulk microphysics. With the binned microphysics we find some crystal losses even for high (~130%) ambient ice supersaturation.

In performing the simulations with the CARMA microphysics we have generally not included surface free energy effects (e.g., Kelvin curvature corrections), which could be potentially important for very small crystals. The treatment of these effects for ice is not as well understood as for water droplets and is complicated by the appearance of many different crystal shapes. We found the implementation of these effects in CARMA to be very sensitive to purely numerical parameters (e.g. time step and bin resolution), motivating its removal at this stage of investigation. This warrants further study, however, because such terms, by making the equilibrium vapor pressure partly dependent on crystal size, can effectively allow large crystals to consume small ones, enhancing the crystal losses found due to the adiabatic heating mechanism alone.

The simulations detailed in Lewellen and Lewellen 2001a extended to contrail ages of 30 minutes. We have conducted preliminary simulations out to contrail ages of 1.5 hours with the LES model including bulk ice microphysics, in order to better assess the problems encountered. In older contrails precipitation can become a significant process in the growth in volume and ice mass of the contrail, even for modest values of the ambient supersaturation with respect to ice. The onset of precipitation within a given region of the contrail is very sensitive to the ice crystal size spectrum there. The study of these effects with the binned microphysics, as well as an assessment of the radiative effects, is deferred for future work.

Given the variety of ambient conditions present in the atmosphere (varied values of temperature, humidity, turbulence level, wind shear, etc.) and different aircraft flying there, a definitive assessment of contrail development and impact involves an exploration in a multi-dimensional parameter space. The current work provides the tools and ground work for such an extensive study in the future.

Recommendations

Since the impact of cirrus clouds remains an important uncertainty in predictions of climate modification, and contrails appear to make a potentially significant contribution to cirrus coverage, at least in local regions, further study of contrail evolution appears warranted. Our current wake code with CARMA ice microphysics provides a unique tool for such investigations. We have considered only a limited range of atmospheric conditions and flight scenarios, and even some of these may profitably be repeated with the latest ice microphysics in the model. Some of the important questions that might be answered in a future grant are:

1. How much difference would a change in flight altitude make in the size of the persistent contrail under some typical atmospheric profiles of humidity, stratification, and wind shear?
2. How sensitive is the evolution of persistent contrails to the uncertainties in small crystal dynamics?
3. For what conditions and at what wake age does ice precipitation and radiation become important to the wake evolution? What are the most important effects of these processes?
4. What interactions between evolving contrails and natural cirrus may be expected to be important?
5. How can the most important features evident from high resolution, 3D simulations be reasonably represented in coarser grid regional or global models?
6. Are there practical strategies for minimizing the occurrence of persistent contrails?

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APPENDIX A

The Effects of Aircraft Wake Dynamics of Contrail Development

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